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FINAL REPORT

Investigation of Ionospheric Particle Interaction

Contract No. AF 19(604)1705

NOVEMBER, 1958

CX - 35A

NEW YORK UNIVERSITY
Institute of Mathematical Sciences
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FINAL REPORT
under
Contract No. AF 19(604)1705

Subject:

Investigation of Ionospheric Particle Interaction

Sidney Borowitz

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Acting Project Director

The research reported in this document has been sponsored by the Geophysics Research Directorate of the Air Force Cambridge Research Center, Air Research and Development Command, under Contract No. AF 19(604)1705.

November, 1958

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FINAL REPORT

Contract Number AF 19(604)1705

This contract, on the investigation of ionospheric particle interaction, was started February 1, 1956 and terminated October 31,1958. Ten reports were issued under the auspices of this contract, most of which have either been published or are about to be published in scientific journals. In addition, two articles were published which were not included as reports. A list of reports and publications is appended.

Summary of the work on the contract

The following were the highlights of the results obtained in reports published for this contract:

The utility of the Kohn-Hulthén variational principle has been improved as a result of work done for this contract both because a principle similar to this one has been derived for the reactance operator as well as for the scattering operator, and because a formulation of this variational principle has been given in which a normalization of the trial function is irrelevant.

We have continued to investigate the many-body problem, with the hydrogen atom as an example, and have succeeded in getting probably the most accurate published value for the scattering of electrons by hydrogen atoms at zero energy. In addition,a novel way of dealing with inelastic processes via the so-called impulse approximation has been formulated and applied to a case of the excitation of a hydrogen atom to its first excited level and to the ionization of hydrogen due to electron impact.

An extension of the WKB approximation to the inelastic scattering of molecules by molecules has been applied to the case of the excitation of the vibrational states of hydrogen by hydrogen impacts. This calculation is not only of intrinsic interest but serves to indicate some of the deficiencies of the previous approximate method for calculating the cross section for these processes (E. Bauer, A Method of Calculating Cross Sections for Molecular Collisions, CX-17).

We have conducted some investigations of the inverse problem, namely the determination of the inverse scattering potential from a knowledge of the cross section. The indications are that this problem even for a fixed potential is so complicated that there is not much hope at present of being able to apply it to the many-body atomic system. However, we will continue to devote a portion of our effort to this type of work.

Finally, we should like to report that the extension of the method of Kato for obtaining upper and lower bounds for scattering phases from a fixed potential has been extended to apply to atomic systems and we expect that good use will be made of this method in the future for evaluating the success of approximate calculations for some of the fundamental cross sections of atomic scatterings.

The work on this contract can be divided into five categories:

I. General scattering theory

Dr. H.E. Moses has succeeded in making the Kohn-Hulthén variational procedure more useful by two reports (CX-26, CX-27) in which simplified versions of this procedure have been derived for the scattering operator and for the reactance operator: a formulation of this principle has been made which is independent of the normalizations of the trial function. This latter procedure has been used by Saxon and Moe in nuclear problems. In CX-30, Professor Spruch has shown how to extend the method originally formulated by T. Kato for obtaining the bounds on scattering phases for the fixed potential to the problem of obtaining bounds on scattering phases for a many-particle problem. Report CX-29 describes the method by which the extension can be carried out. We are in the process of applying this to actual atomic systems (see work in progress at the end of this report).

II. Many-particle scattering problems

During the contract period we have continued to use as a model for a many-particle scattering system the scattering of electrons by hydrogen atoms, with the hope that by a careful analysis we will obtain some general results applicable to the scattering by more complicated atomic systems. In Report CX-29 Dr. Greenberg and Professor Borowitz have made a careful and what is believed to be an accurate calculation of the zero energy scattering of electrons by hydrogen atoms. These results do not differ appreciably from the scattering of the incoming electron by the static potential of the hydrogen atom. In CX-34 a novel way of calculating the inelastic scattering of electrons by hydrogen atoms has been formulated and applied. The idea in this paper is to consider the hydrogen atom as frozen during the scattering process and then to average over the initial and final states of the electron, superimposing the effect of the Coulomb scattering of the electron. We are fortunate in this case to find experimental results with which the theory can be compared very favorably. The general result is that we have much less labor and much more accurate results than would be obtained with the second Born approximation.

III. Molecular vibrations in collisions

In report No. CX-31 Drs. M. Salkoff and E. Bauer have calculated the excitation of molecular vibrations by the collision of hydrogen molecules with hydrogen molecules. The interesting features of this report have been that for the first time the WKB approximation has been used for the calculation of inelastic processes. In addition, the extensive numerical calculations in this report indicate that previous methods of calculating the excitation of molecules by molecules have been in error. In particular, the use of the Born approximation gives results which are altogether incorrect,at least in the hydrogen molecule case.

IV. Molecular wave functions

This contract has partially supported a rather extensive activity in the calculation of the intermolecular potentials for the ground state and excited states of diatomic molecules. (The rest of this program has been supported by the NACA.) This program has, to date, been engaged in calculating on the IBM 704 machine at New York University a set of tables which will simplify the evaluation of an Exchange,Coulomb, and Many-centered integrals which occur in the Hartree calculations of intermolecular potentials. In Report CX-35 Dr. C. Donald La Budde and R.C. Sahni put forth an improved method for the convergence of two and three-center integrals.

V. Miscellaneous

In CX-28 Dr. Bauer has calculated the transition probability of transfer of energy from one optic mode to two or three acoustic modes of vibration for sodium chloride at low temperatures. In CX-33 Dr. Bauer has written a survey article on chemical exchange reactions involving relatively light atoms. He has indicated how one might set about calculating such reaction rates in situations where the usual classical statistical theory of chemical reaction is not applicable. He has shown how one could use a more adequate knowledge of the interatomic potential energy function in the calculation of such rays. Finally, in CX-32, Drs. H.E. Moses and I. Kay have investigated the determination of the scattering potential from a class of potentials in which the poles of the scattering matrix do not correspond to real bound states of the system.

Work in progress

At the conclusion of this contract there is a considerable amount of work in progress which of course has not been published in reports. We intend to continue this work in our research program on atomic scattering at New York University.

One class of problem has been the method of obtaining a simple expression for approximate wave functions for the many-body problem as applied to light atoms. Two methods have been used. One is to deduce the best type of correlated wave function by assuming certain simple types of wave functions somewhat more complicated than Hartree-types and to use a variational principle for determining the best functional form of these wave functions. The other method has been to use products of one electron wave functions times a Bessel function of a particular form in the interelectron coordinate. The latter method has been applied to the case of lithium and gives a result very close to the experimental one for the lowest bound state energy. Another type of investigation has been in connection with the many-body scattering problem. Here the objective has been two fold, generalizing the Hartree-Fock approach, and 2), to find some scheme for reproducing the experimental maximum at three electron volts which Bederson and his collaborators have found in the scattering of electrons by hydrogen atoms. Another line of investigation which has just been undertaken is to find a way of generalizing the Thomas Fermi model to describe excited electronic states. We have also been doing some work in general scattering theory. One attack has been to gain some familiarity with the Watson transformation - a technique which we have applied to the scattering of very fast electrons by a Coulomb potential, in cases where the relativistic affect is important. We are now using this same Watson transformation as the start of a perturbation procedure when one has an infinitely repulsive core. This type of problem occurs when we consider the collisions of molecules with molecules and also has applicability to nuclear physics since one model gives an infinite repulsive core for the internuclear potential. Also the method of obtaining upper and lower bounds for scattering phases is being applied to the scattering of low energy electrons and positrons by hydrogen atoms. Finally, we are investigating the feasibility of using the IBM 704 machine to construct an exact solution of the problem of the scattering of electrons by hydrogen atoms.

This contract has partially supported three graduate students during their research work toward the Ph.D. degree.

Research Reports and Publications

The following is a list of all research reports in the CX series.

Under Contract No. AF 19(122)-463

CX-1	S. Borowitz	The Schwinger Variational Method for Three-Body Collisions Published - Borowitz and Friedman, Phys. Rev., 89, 441 (1953).	April, '52
CX-2	H. Moses	A Self-Consistent Calculation of the Dissociation of Oxygen in the Upper Atmosphere Published - Phys. Rev., 87, 628 (1952).	April, '52
CX-3	K. Wildermuth	A Rigorous Solution of a Many-Body Problem Published - Acta Physica Austriaca, 7, 299 (1953).	Aug. '52
CX-4	B. Friedman and E. Gerjuoy	Scattering Problems in Nonrelativistic Quantum Mechanics; Part I - One Particle in One Dimension	Dec. '52
CX-5	H. Moses	Exchange Scattering in a Three-Body Problem Published - Phys. Rev., 91, (1953). Math. Rev., 16, 1186 (1955).	Jan. '53
CX-6	H. Moses	Formulation of the Kohn-Hulthén Variational Principle in Terms of the Scattering Operator Formalism Published - Phys. Rev., 92, 817 (1953). Math. Rev., 15, 587 (1954).	April, '53
CX-7	H. Boyet and S. Borowitz	A Variational Calculation of the Elastic Scattering of Electrons by Hydrogen Atoms Published - Phys. Rev., 93, 1225 (1954).	April, '53
CX-8	H. Moses	A Self-Consistent Calculation of the Dissociation of Oxygen in the Upper Atmosphere; Part II - Three-Body Recombinations Published - Phys. Rev., 91, 1408 (1953).	April, '53

CX-9	E. Bauer and Ta-You Wu	The Origin of the E-Layer of the Ionosphere Published - Phys. Rev., 92, 1101 (1953).	July, '53
CX-10	J.B. Keller	Derivation of the Bohr-Sommerfeld Quantum Conditions from an Asymptotic Solution of the Schrödinger Equation Published - Annals of Physics, 4, No. 2, 180 (1958).	July, '53
CX-11	E. Bauer	Self-Consistent Field Equations for H_2 and H_3	Aug., '53
CX-12	H. Moses	The Scattering Operator in Quantum Mechanics, Part I - The Properties of the Scattering Operator from the Time-Dependent Schrödinger Equation (see CX-13) Math. Rev., 16, 1186 (1955).	Oct., '53
CX-13	H. Moses	The Scattering Operator in Quantum Mechanics - Part II - The Scattering Operator Formalism and Other Formalisms Published - (CX-12 and CX-13, portion of the material) - Phys. Rev., 96, 519 (1954). Published - (CX-12 and CX-13, summary) - Il Nuovo Cimento, 1, 103 (1955). Math. Rev., 16, 1187 (1955).	Dec., '53
CX-14	E. Bauer and Ta-You Wu	The Cooling of a Gas by Radiation Published - Proc. Phys. Soc. of London, A 67, 741 (1954).	April, '54
CX-15	S. Schwebel	An Evaluation of Approximation Methods for Three-Body Scattering Problems Published - Phys. Rev., 103, 814 (1956). Math. Rev., 16, 1187 (1955). Math. Rev., 18, 701 (1957).	May, '54
CX-16	S. Borowitz	A Perturbation Calculation of the Elastic Scattering of Electrons by Hydrogen Atoms Published - Phys. Rev., 96, 1523 (1954).	June, '54

CX-17	E. Bauer	A Method of Calculating Cross Sections for Molecular Collisions Published - J. Chem. Phys., 23, 1087 (1955).	Oct., '54
CX-18	H. Moses and I. Kay	The Determination of the Scattering Potential from the Spectral Measure Function Math. Rev., 17, 372 (1956). Published - Il Nuovo Cimento, 2, 917 (1955). Math. Rev., 16, 929 (1955). Math. Rev., 17, 372 (1956).	Jan., '55
CX-19	H. Moses and I. Kay	The Determination of the Scattering Potential from the Spectral Measure Function, Part II - Point Eigenvalues and Proper Eigenfunctions Math. Rev., 17, 155 (1956). Published - Il Nuovo Cimento, 3, 66 (1956). Math. Rev., 17, 740 (1956).	June, '55
CX-20	H. Moses and I. Kay	The Determination of the Scattering Potential from the Spectral Measure Function, Part III - Calculation of the Scattering Potential from the Scattering Operator for the One-dimensional Schrödinger Equation Published - Il Nuovo Cimento, 3, 276 (1956). Math. Rev., 17, 489 (1956).	Sept., '55
CX-21	E. Bauer and Ta-You Wu	Dissociative Recombination Published - Canadian J. of Phys., 34, 1436 (1956).	Oct., '55
CX-22	S. Borowitz and M. Klein	A Perturbation Calculation of the Inelastic Scattering of Electrons by Hydrogen Atoms Published - Phys. Rev., 103, 612 (1956).	Nov., '55
CX-23	B. Zumino	On the Formal Theory of Collisions and Reaction Processes	Mar., '56
CX-24	L. Spruch	On the Eigenvalues Which Give Upper and Lower Bounds on Scattering Waves Published - Phys. Rev., 109, 2144 (1958). Math. Rev., 17, 1088 (1956).	April, '56

CX-25	T. Kato	On the Eigenvalues of Many-Particle Systems in Quantum Mechanics Published - Comm. Pure and Appl. Math., 10, 151 (1957). Math. Rev., 17, 1260 (1956).	April, '56

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CX-26 (AD98707)	H. Moses	The Kohn-Hulthén Variational Procedure for the Scattering Operator and the Reactance Operator, Part I: Elementary Form of the Variational Principle Published - Il Nuovo Cimento, 5, 120 (1957). Math. Rev., 18, 540 (1957).	June, '56
CX-27 (AD98722)	H. Moses	The Kohn-Hulthén Variational Procedure for the Scattering Operator and the Reactance Operator, Part II: Procedures Independent of the Normalization of the Trial Functions Published - Il Nuovo Cimento, 5, 144 (1957). Math. Rev., 18, 540 (1957).	July, '56
CX-28 (AD110229)	E. Bauer	Coupling of Optic and Acoustic Modes of Vibration in Crystals Published - J. Chem. Phys., 26, 1440 (1957). Math. Rev., 18, 612 (1957).	Sept., '56
CX-29 (AD117246)	H. Greenberg and S. Borowitz	A Variational Calculation of the Scattering Cross Section for Nearly Zero Energy Electrons by Hydrogen Atoms Published - Phys. Rev., 108, 716 (1957).	April, '57
CX-30 (AD117247)	L. Spruch	Bounds on Scattering Phase Shifts Published - Phys. Rev., 109, 2149 (1958).	May, '57
CX-31 (AD133673)	M. Salkoff and E. Bauer	Excitation of Molecular Vibration by Collision Published - J. Chem. Phys., 29, 26 (1958).	July, '57
CX-32 (AD133810)	I. Kay and H. Moses	The Determination of the Scattering Potential from the Spectral Measure Function- Part IV: 'Pathological' Scattering Problems in One-Dimension Published - Il Nuovo Cimento, 5, 230 (1957).	Sept., '57

CX-33 (AD152496)	E. Bauer	Quantum Theory of Chemical Reaction Rates	Mar., '58
CX-34	R. Akerib and S. Borowitz	The Application of the Impulse Approximation to the Inelastic Scattering of Electrons by Hydrogen Atoms Submitted - Phys. Rev.	July, '58
CX-35	C.D. LaBudde and R.C. Sahni	The Evaluation of Two and Three-center Integrals Arising in Calculations on Molecular Structure	Sept., '58

List of Publications not Based on Reports

S. Borowitz and B. Friedman	Three-Body Scattering Problems Phys. Rev., 93, 251 (1954).
S. Borowtiz	Electron-Ion Recombination at Low Pressures; Trans. AIEE, 72, Part I: 430 (1953).
H. Moses	Calculation of the Scattering Potential from Reflection Coefficients Phys. Rev., 102, 559 (1956).
J. Keller, I. Kay and J. Shmoys	Determination of the Potential from Scattering Data Phys. Rev., 102, 557 (1956).
J. Keller	Bounds on Phase Shifts Published - Il Nuovo Cimento, 5, 1122 (1957).
H. Moses	Pathological Scattering in One Dimension Published - Il Nuovo Cimento, 5, 230 (1957).
E. Bauer and T.Y. Wu	Thermal Expansion of a Linear Chain Phys. Rev., 104, 914 (1956).

Date Due

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Borowitz.
Final report under Contract No. AF 19(604)1705: Investigation of ionospheric particle interaction.

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